RESEARCH INTO BORON-CARBON NANOTUBE MODIFIED BY ALKALINE METAL ATOMS

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We studied the mechanism of Li, K and Na atoms sorption on the external surface of single-walled BC_5 nanotubes. We defined the optimal geometry of the sorption complexes and obtained the sorption energy values. The analysis of the band gap structure suggests that the band gap is insensitive to adsorption process. The electron density is located near the surface atoms of the tube.

The boron carbon nanotube (6,0) has been chosen as a main object of the research. The borders of the nanotube modified with hydrogen pseudo atoms for compensation of the unsaturated chemical bonds. The calculations has been carried out using molecular cluster model and Density Functional Theory (DFT) method [1-4].

For avoiding the border effects, the sorption centers located in the middle of the nanotube. The calculation has been carried out using reaction coordinate method. The approaching step has been chosen equal to the 0,1 A along the perpendicular to the longitude axis of the nanotube. All geometry parameters has been optimized during the calculation process. After the calculation, the adsorption energy and distance have been carried out. The adsorption energy and sorption distance for obtained processes are presented on the figure 1.

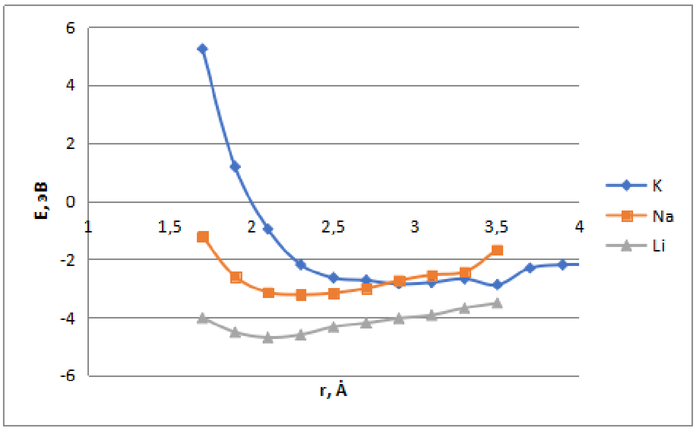

Fig. 1. Potential energy curves of the interaction process for BC nanotube and alkali metal atoms

The adsorption energy has been calculated using equation 1:

$$E_{ад} = E_{ад.к.} - (E_{tub} + E_{Li,K,Na}) \qquad (1)$$

where $E_{ад}$ – adsorption energy; $E_{ад.к.}$ – the energy of the obtained complex; E_{tub} – the nanotube energy; $E_{Li,\ K,\ Na}$ – the metal atom energy.

The charge distribution over the metal atoms indicates that electron transfer to boron and carbon atoms located on the nanotube external surface takes place, which increases the number of majority charge carriers in tubulenes; as a result BC_5 nanotubes, which we had previously classified as narrow-gap semiconductor, begin to take on metallic properties (the occurrence of surface conductivity is attributed to electrons from metal atoms)

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INVESTIGATION OF EFFICIENCY INCREASING FOR PACKING COLUMNS USING CARBON NANOTUBES

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The aim of this paper was to investigate the possibility of selectivity increasing for packing columns with carbon nanotubes (CNT). For this purpose we used three types of columns: pure CNT, pure Plate (siliceous gel), mixture of plate and CNT. As analyzed materials three organic compounds have been chosen: hexane, acetone, benzol. The results of the analysis showed, that pure CNT couldn't be used for the chromatography, but adding them in the plate made the selectivity process more effective.

Carbon nanotubes due to the feature properties [1-4], have unique sorption properties. The structure which represents the decanter monolayer curtailed into a tube gives to material very high rate of a specific surface [5]. This indicator is one of the main in the choice of a sorbent of a motionless phase for a gas adsorption chromatography. Therefore, use of tubulen in a nozzle column can raise relevance of the last and compete with capillary columns [6,7].

For comparison of dividing ability of columns it was decided to use values of volumes of keeping of the divided substances at various temperature of columns. The volume of keeping is on a formula:

$$V_r = a * t_r\ [ml]$$

where a — the speed of gas carrier (ml/c), t_r — time of keeping of the divided component (c).